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Modeling of Ultrafast Laser Induced Electron Emission from TI and Graphene

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Final Report for AOARD Grant FA2386-14-1-4020

Modeling of Ultrafast Laser Induced Electron Emission from Graphene and Topological Insulator

Date: 15 July 2017

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Abstract:
The most important outcome of this grant is a comprehensive revision of the traditional electron emission theories which were developed decades ago, in order to include the unique properties of two-dimensional (2D) materials like graphene. From the scientific findings, new scaling laws are reported and potential applications such as energy harvesting are suggested.

Introduction:
Since the discovery of large size graphene in 2004, it has initiated very active research activities in understanding the unique electronic properties of graphene, including high carrier mobility, ballistic transport, and linear light-like energy dispersion relationship. Promising applications include field effect transistors, sensors, spintronic devices, and many others in nano-electronics. Graphene is also a good cathode material to emitted current required for many applications such as electron source for high power microwave source. Recent experiments have also indicated ultrafast laser are useful to emit high electron bunches for the similar applications. In this proposal, the objectives are to provide a comprehensive theoretical study to revise various electron mechanisms (field emission, thermionic emission, photoemission and space charge limited emission) that the traditional models may not valid due to the nature of 2D materials. In additional to scientific findings, we will also focus on exploring new applications that resulted from the new emission models discovered. While the focus of the studies is on graphene, but the findings reported should be valid for other 2D materials as long as there is a linear energy dispersion,

Approaches:
For our theoretical models, we started from solving the consistent coupled equations involving Maxwell, Schrodinger and Dirac equations. The approach is similar to the prior formulation but we now explicitly include the properties of 2D materials, such as linear energy dispersion in our model. Our model is aimed to be universal and general that it can recover to the traditional models. Thus it has the advantages of study mesoscopic materials. If possible, we will compare our calculated results with other experimental results or suggest a clear experimental setting or design parameters in order for further verification.

Results and Discussions:
As mentioned before, we are the first group in performing this complete revision and some new scaling laws have been reported for the first time with 10 journal papers have been published in past 3 years. Due to its importance, the PI was recently invited to write a not-so technical article published the Material Research Society (MRS) bulletin (July 2017 issue). A review paper of space charge limited current was also published in the Applied Physics Review (March 2017 issue) to review the advancement of this topic in past 100 years.

From our works, the results are not only valid for electron emission from 2D materials to free space, but also applicable for electron injection from 2D materials to another solid, which may provide some basis to study the electric contact of 2D materials. Thus the famous Schottdy diode equation for a graphene-semiconductor has been reported in the most recent prestigious conference in electron device: IEDM in San Francisco (Dec 2016): 4 papers accepted from Singapore and 7 papers each from MIT and Stanford. The finding was also reported by the semiconductor-today online:

http://www.semiconductor-today.com/news_items/2017/jan/sutd_040117.shtml

The first paper published in 2015 [Shijun Liang, and L. K. Ang, "Electron Thermionic Emission from Graphene and thermionic energy convertor", Phys. Rev. Applied 3, 014002 (2015)] was reported in the following websites. Shijun Liang recently just completed his PhD degree in SUTD.

- http://www.nanowerk.com/spotlight/spotid=39283.php
- http://www.greencarcongress.com/2015/03/20150309-sutd.html
- http://nanotechweb.org/cws/article/yournews/60434

Based on these results, the PI has recently secure a 3 years funding in Singapore (June 2017 – June 2020) to further study the application of these electron emission models to study the electrical contact problem between 2D materials and the traditional bulk materials and/or other novel materials such as superconductors and Weyl semimetals. Many scaling laws predicted are also pending for further verification. Some new applications (energy harvesting and photo-detectors) proposed in this grant will also be explored for other funding in collaboration with experimental groups. In particular, the paper [S. J. Liang, Bo Liu, Wei Hu, Kun Zhou and L. K. Ang, Thermionic Energy Conversion Based on Graphene van der Waals Heterostructures, Scientific Report 7:46211 (2017)], was highlighted in the graphene-info website:

https://www.graphene-info.com/researchers-singapore-design-graphene-based-high-efficiency-energy-harvesting-device

The PI currently has 4 PhD students (2 co-supervision with experimentalists) to work on these future works.

In the following, we briefly describe some important findings according to the publication list (see below). The details can be found in the attached papers.

1. New models of electron emission from graphene
   This invited paper provides a non-technical review - published in MRS bulletin (a magazine like)

2. Relativistic space charge limited current transport in 2D materials
   This paper shows that the traditional scaling of V^2/L^3 (V = voltage, L = diode length) is not valid for 2D materials. A new model is created consistently and will be useful to determine the mobility of 2D materials and also able to explain the "unexpected experimental results" reported by others.

3. Thermionic Energy Conversion Based on Graphene van der Waals Hetero-structures
   This paper shows that it is possible to harvest waste heat at low temperature (400 K to 500 K) making use of the electron thermionic emission from graphene electrode into vdW hetero-structure.

4. Review of space charge limited current
   Collaborated with other groups, a long paper is written to review the past advances in 100 years.

5. Schottky contact model for graphene-semiconductor contact
   This IEDM paper reports a correct contact model for graphene-semiconductor interface. Models are compared with experimental results from Italy

6. Guide modes in graphene based waveguide
   The electron transport in graphene follows Dirac equation – which is analogous to wave equations. Thus a graphene-based electron waveguide is studied in this paper.

7. Current-temperature scaling for a Schottky interface with non-parabolic energy Dispersion
   This paper shows a smooth transition of the 2 temperature scalings: T^2 (bulk materials) and T^3 (2D materials). It is an extension of prior work in #11.

8. Protrusive Child-langmuir (CL) law
   This papers shows the new fractional modeling of space charge limited current from rough cathode

9. Graphene-plasmon created by inelastic electron tunneling
   This paper reports a new way to generate graphene plasmons by using in-elastic electron tunneling and to report the advantages of using graphene as compared to metals at longer wavelength.

10. Space charge limited (SCL) current for a sharp tip
    This paper produces a model to account for SCL current emitted from a sharp tip

11. New Temperature scaling of thermionic emission from graphene
    This paper reports the current temperature scaling of T^3 as compared to the traditional T^2 scaling derived by Richard-Dushman law many decades ago.

List of Publications and Significant Collaborations that resulted from your AOARD supported project: 10 Papers published in peer-reviewed journals and 1 peer-revised conference proceeding

1. Y. S. Ang, S. J. Liang and L. K. Ang, Theoretical Modelling of Electron Emission from Graphene, MRS Bulletin 42, 505 (10 July 2017) – invited paper
2. Y. S. Ang, M. Zubair, and L. K. Ang Relativistic space charge limited current for massive Dirac fermions, Phys. Rev. B 95, 165409 (2017)
3. S. J. Liang, Bo Liu, Wei Hu, Kun Zhou and L. K. Ang, Thermionic Energy Conversion Based on Graphene van der Waals Heterostructures, Scientific Report 7:46211 (2017)
4. P. Zhang, A. Valfells, L. K. Ang, J. W. Luginsland and Y. Y. Lau, 100 years of the physics of diodes, Applied Physics Reviews 4 011304 (3/2017) – review paper
5. S. J. Liang, W. Hu, A. Di Bartolomeo, S. Adam and L. K. Ang A modified Schottky model for graphene-semiconductor (3D/2D) contact: A combined theoretical and experimental study, paper #118240, 2016 IEEE International Electron Device Meeting (IEDM), San Francisco, CA USA 5 to 7 December (2016)
6. Y. Xu and L. K. Ang, Guided Modes in a Double-Well Asymmetric Potential of a Graphene Waveguide, Electronics 5, 87 (2016) – free open access journal
7. Y. S. Ang, and L. K. Ang, Current-temperature scaling for a Schottky interface with non-parabolic energy Dispersion, Phys. Rev. Applied. 6, 034013 (2016)
8. M. Zubair, and L. K. Ang Fractional-dimensional Child-Langmuir law for a rough cathode, Phys. Plasmas 23, 072118 (2016)
9. Kelvin. J. A. Ooi, H. S. Chu, C. Y. Hsieh, Dawn T. H. Tan, and L. K. Ang, Highly Efficient Midinfrared On-Chip Electrical Generation of Graphene Plasmons by Inelastic Electron Tunneling Excitation, Phys. Rev. Applied. 3, 054001 (2015)
10. Y. B. Zhu, and L. K. Ang Space charge limited current for a sharp tip, Phys. Plasmas 22, 052106 (2015)
11. S. J. Liang, and L. K. Ang, Electron thermionic emission from graphene and a thermionic energy converter, Phys. Rev. Applied. 3, 014002 (2015)

List any interactions with industry or with Air Force Research Laboratory (AFRL) scientists: AOARD window of science award to visit 2 AFRL labs and gave presentation in 2015 -

L. K. Ang “Ultrafast laser induced electron emission, and electron emission from graphene”, AFRL lab, Dayton, USA, 10 July (2015). Hosted by Dr. Steven B. Fairchild

L. K. Ang “Ultrafast laser induced electron emission, space charge limited current and electron emission from graphene”, AFRL lab, ABQ, USA, 7 July (2015). Hosted by Dr. Wilkin Tang